Monte Carlo Minimization of the Higgs-Landau Potentials

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We propose a Monte Carlo algorithm to search for the boundary points of the orbit space which is important in determining the symmetry breaking directions in the Higgs potential and the Landau potential. Our algorithm is robust, efficient and generally applicable. We apply the method to the Landau potential of the $d-$wave abnormal superconductor.

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I. INTRODUCTION

There are many branches of physics where the symmetry breaking is important yet its analysis is highly non-trivial. The Higgs potential and the Coleman-Weinberg potential in the unification theories are difficult to minimize except for simple cases. Extremization of the superpotential in the supersymmetric unification theories is non-trivial. The Landau potential in many branches of condensed matter physics is often times tricky to handle.

The Michel-Radicati conjecture [1] that a group invariant potential has extrema at a few critical strata corresponding to the maximal little groups was handy and utilized by many model builders [2,3]. The group theoretical method allows one to locate the extrema from the list of maximal little groups without solving the coupled third degree extremum equations. It stirred up considerable research efforts. Slansky [2] made lengthy tables of little groups of many representations that could be used in the grand unification model building. Abud and Sartori [4] ellaborated the geometrical structure of the strata of an irreducible representation. Stokes and Hatch [5] made a complete set of tables for the isotropy groups of the irreducible representations of 230 space groups. However, Tolédano's [6] found counter-examples to the conjecture. Moreover, the conjecture is less useful for a reducible representation where strata of maximal little groups are oftentimes not one-dimensional critical strata.

Some years ago one of the authors [7,8] devised an efficient method for finding symmetry breaking directions in those problems. His method was practical and could be used for any representations. The key point in the method was the concept of the orbit parameters, which are defined to be the dimensionless ratios of (*polynomial or non-polynomial*) invariant functions to the unique isotropic quadratic invariant. For a reducible representation the ratio is taken over the product of quadratic invariants of each irreducible representation. Thus an orbit parameter is a kind of angular parameter. The space of such orbit parameters occupies a confined region, which is called the orbit space. Being defined out of invariants each point in the orbit space remains unchanged by the symmetry operations and has a definite residual symmetry associated with it, its little group, or sometimes called the isotropy group. Kim showed that the most general quartic Higgs or Landau potential has the absolute minimum at the most protruding point of the orbit space, which corresponds most likely to one of the critical strata in the case of an irreducible representation but not necessarily so in the case of a reducible representation. He showed that if the Michel-Radicati conjecture is to be valid the orbit space boundary has to be concave except at the cusps corresponding to the critical strata. Once the orbit space is constructed then the minimization of the potentials and the identification of symmetries are easy. One can easily identify the minimum point, simply by a look at the orbit space in the two dimensional case.

The advantage of this method is that it finds not only the critical strata of maximal little groups but also non-critical strata of submaximal little groups and the phase diagram can be constructed easily. It is powerful if used with the extensive tables made by Slansky [2] and Hatch and Stokes [5]. It is most useful when the representation dimension is large and the orbit space dimension is two or three.

It has been known [9,10] that the orbit space is a bounded object with a hierarchical structure. The points corresponding to the higher symmetries lie hierarchically closer to the surface of the orbit space and the interior points correspond to the unique lowest symmetry. The points of higher symmetries always form the boundaries of those of lower symmetries. The isolated points corresponding to the highest symmetries are zero dimensional objects and thus the derivatives of the orbit parameters with respect to the elements of the representation vector, sometimes called the carrier space vector, are zero. Thus the Michel-Radicati conjecture is a natural consequence of the orbit space structure and thus a group invariant function always has extrema on the critical strata [11]. There are additional

extrema which depend on the particular choice of the invariant potential. In order to determine the absolute minimum one has to compare all these local extrema. Thus one has to get the full orbit space boundary to locate it.

Nobody showed that the orbit space boundary of an irreducible representation is concave except at the cusps. It is more likely that a high dimensional representation has many convex boundary portions as the number of available maximal little groups are limited. Moreover, the boundaries of an orbit space of a reducible representation have many convex boundaries [7]. Nevertheless one can use this group theoretical property and systematically search for the little groups and the corresponding invariant directions to construct the orbit space [2,5]. Several examples were illustrated in [4,12,13].

One often times deals with the projected subspace of the full orbit space. With respect to the subspace the above hierarchy theorem does not necessarily hold. When the symmetry group is a non-simple group it is awkward to make a list of isotropy groups and the associated invariant directions. In this case the above theorem seems to be much less useful. Also when the dimension of the representation is large it is non-trivial to find the invariant directions corresponding to the little groups.

II. MONTE CARLO SEARCH OF THE ORBIT SPACE

Thus it is necessary to have an alternative method for building the orbit space. Simple Monte Carlo methods that were tried in the past [7,4] were not efficient for obtaining the orbit space boundary. We have devised a more efficient Monte Carlo method for building the orbit space. It is applicable to any representation and robust. The algorithm uses the von Neumann rejection method [14] and the over-relaxation method.

Suppose that we are searching for the boundary curves of a two-dimensional orbit space, (θ, ϕ). Let us assume that the orbit parameters θ and ϕ are functions of M variables, x_m. Then our algorithm is stated as follows:

(1) Initially N points are sampled in a uniformly random way. That is, N sets of x_m are sampled in a uniformly random way from the interval [-1, 1]. Then one computes the center of gravity, (θ_C, ϕ_C), of these N points, (θ_i, ϕ_i).

(2) For the N points, one computes the angle of the vector, $(\theta_i - \theta_C, \phi_i - \phi_C)$ and assigns an angular bin. Let the total number of bins be D.

(3) One then identifies the outermost points along each of the D discrete directions. The 'outwardness' is defined to be the distance of the point from the center of gravity.

(4) Starting from each of these selected points, a random walker with $M-$legs makes moves by moving one of its legs, x_m. If the move increases the distance, it is accepted. If not, the random walker steps the leg in the opposite direction with a different stride. If the move increases the distance, it is accepted. Otherwise it is rejected and the old value of x_m is retained.

If the random walker jumps over into another angular bin, its position is compared with the current outermost point along that direction. The more distant of the two is selected as the new outermost point in that angular bin.

(5) Step 4 is repeated for all x_m.

(6) Step 4 and 5 are repeated along all the angular directions.

(7) Step 4, 5 and 6 are repeated a finite times Rt or until no further appreciable improvements are made within the allowed number of trials.

(8) The search of the orbit space boundary is completed.

The circumference of the orbit space is discretized into D bins and the outermost point in each bin is sought after. In the random search for the boundary points the random walker of a selected bin is encouraged when it moves towards the surface. If a move $x_m \to x_m + \delta$ is unsuccessful then another move $x_m \to x_m - \omega \cdot \delta$ is tried, where ω is an adjustable relaxation parameter. Even when the random walker strays into another direction its move is not discarded but compared with the current outermost point. In this way the random walker finds the outward direction in most attempts. Therefore the convergence rate is very fast.

III. APPLICATIONS

Recently there have been some activities to search for anisotropic superconductivity [3]. It has been confirmed that a d-wave pairing actually occurs [15]. We have been investigating a model of an abnormal superconductor with the high temperature symmetry [16], $G \equiv O(3) \times U(1) \times T$. For the spin-0 $d-$wave gap functions the 3-dimensional symmetric traceless complex matrix, Φ_{ij}, is assumed for the order parameter. Under $O(3)$ the indices i, j transform like a three dimensional vector. The $U(1)$ transforms $\Phi \to e^{i\lambda}\Phi$ and $\Phi^* \to e^{-i\lambda}\Phi$. The time reversal symmetry T transforms $\Phi \to \Phi^*$ and vice versa.

Then the most general Landau potential upto the fourth degree in Φ can be written as a polynomial of the basic invariant polynomials.

$$V(\Phi) = \alpha I_0 + \beta I_0^2 + \gamma_1 T_1 + \gamma_2 T_2 \tag{1}$$

Each basic invariant polynomial is defined as follows:

$$I_0 = \Phi_{ij}\Phi^*_{ji} \tag{2}$$

$$T_1 = \Phi_{ij}\Phi^*_{jk}\Phi_{kl}\Phi^*_{li}, \quad T_2 = \Phi_{ij}\Phi_{jk}\Phi^*_{kl}\Phi^*_{li} \tag{3}$$

where repeated indices imply summation from 1 to 3. It is obvious that these are invariant under the symmetry group G.

The orbit parameters, θ and ϕ are defined as:

$$\theta \equiv \frac{T_1}{I_0^2}, \quad \phi \equiv \frac{T_2}{I_0^2} \tag{4}$$

Along the chosen direction (θ, ϕ), the Landau potential has a directional minimum value,

$$V_0(\theta, \phi) = -\frac{1}{4}\frac{\alpha^2}{(\beta + \gamma_1\theta + \gamma_2\phi)} \tag{5}$$

and the absolute minimum occurs along a direction where $(\beta + \gamma_1\theta + \gamma_2\phi)$ has the smallest value.

By choosing an appropriate basis, we can always have one of the two real matrices in a diagonal form. So there are actually 7 independent components in Φ_{kl}. We can define these 7 independent components like:

$$\Phi_{kl} \equiv \begin{pmatrix} a & 0 & 0 \\ 0 & b & 0 \\ 0 & 0 & -a-b \end{pmatrix} + i \begin{pmatrix} s & u & v \\ u & t & w \\ v & w & -s-t \end{pmatrix} \tag{6}$$

We have run the program with the set of parameters: $N = 2100$, $Rt = 7$, $D = 360$, $\delta = 0.125$ and $\omega = 0.1$. The acceptance rate was 0.460. The result of the run is as shown in Fig. 1. The orbit space, (θ, ϕ), is a triangle with vertices at P1=(1.0,0.0), P2=(0.5,0.5), and P3=$(0.\dot{3},0.\dot{3})$. P1 is associated with the set of variables, $(a = 1, b = -1, s = t = 0, u = 1, v = w = 0)$, and its little group is $D_{4h} \times e^{i\pi} \times T$. P2 is overlapped by two cusps, $\mathrm{p}_2 = (a = 1, b = 1, s = t = u = v = w = 0)$ corresponding to $O^z(2) \times T$ and $\mathrm{p}_4 = (a = 1, b = -1, s = t = u = v = w = 0)$ corresponding to $D_{4h} \times e^{i\pi} \times T$. P3 is associated with $(a = 1, b = Q, s = Q, t = 1, u = v = w = 0)$ where $Q = -2 - \sqrt{3}$ corresponding to the little group $D_{4h} \times e^{i\pi/2} \times T$.

The little groups of these points are maximal isotropy groups of the high temperature symmetry G. The spacial part of the isotropy groups of P_1, P_3 and P_4 are all D_{4h} but their embeddings in G are all different. The elements of these subgroups are listed, in terms of the symbols used in the *International Tables for X-ray Crystallography*, as follows:

$$\begin{aligned} H(P_1) = \; & \{R_1, R_2, R_9, R_{10}\}, \\ & \{R_3, R_4, R_{11}, R_{12}\} \times e^{i\pi}, \\ & \{R_5, R_6, R_{13}, R_{14}\} \times T, \\ & \{R_7, R_8, R_{15}, R_{16}\} \times e^{i\pi} \times T \end{aligned} \tag{7}$$

$$H(P_2) = O^z(2) \times T \tag{8}$$

$$H(P_3) = \{R_1, R_2, R_5, R_6, R_9, R_{10}, R_{13}, R_{14}\}, \\ \{R_3, R_4, R_7, R_8, R_{11}, R_{12}, R_{15}, R_{16}\} \times e^{i\pi/2} \times T \tag{9}$$

$$H(P_4) = \{R_1, R_2, R_5, R_6, R_9, R_{10}, R_{13}, R_{14}\} \times T, \\ \{R_3, R_4, R_7, R_8, R_{11}, R_{12}, R_{15}, R_{16}\} \times e^{i\pi} \times T \tag{10}$$

The Landau potential (1) truncated at the fourth degree can have no lower symmetry than those of these four points [7,8]. The degeneracy at P2 can be lifted if we include the sixth degree terms. (see Fig. 2)

It is interesting that the orbit space has a *convex* boundary portion in the subspace defined by ϕ and $\xi \equiv (\Phi_{ij}\Phi^*_{jk}\Phi_{kl}\Phi_{lm}\Phi^*_{mn}\Phi^*_{ni})/I_0^3$. It is shown in Fig. 2. This implies that if we include the relevant sixth degree term in the Landau potential non-maximal symmetries may be observed at low temperatures depending on the stengths of the expansion coefficients.

IV. DISCUSSIONS

For a $d-$dimensional orbit space, the distance measure is defined in the same way, i.e., the distance from the random walker's position to the center of gravity. In three dimensions, if the whole range of the two angles, polar and azimuthal, are divided into 180 and 360 bins, then the number of bins alone is huge, 64800. For even higher dimensions binning the directions is out of the question. We will need an adaptive Monte Carlo method in this case. Namely, we allocate more random walkers in regions of interest. However, cusps can be found easily with only a few bins.

There are several parameters that the user selects, the number of angular bins D, the initial number of points N, the number of repeats Rt, the random walker's stride δ, and the relaxation parameter ω. The optimum choice of these parameters can only be found empirically.

We tested our method using several Higgs potentials and the Landau potential of ^{3}He. First of all, the outcome depends on the choice of the center of gravity heavily. So we cannot sensibly give a performance report in a neat table of numbers. We found that N and Rt must be selected in proportion to the dimension M of the representation. A large value of D may yield sharper boundary curves but it need not be larger than 360. Cusps could be obtained very easily even with very small D.

The random walker has to pass many singular curves on its march towards the surface. These curves are orbits of submaximal isotropy groups. They are on the boundary surface in the full orbit space and the Jacobian of the orbit parameters with respect to x_m vanishes along those curves [7]. In the projected orbit space parts of the curves are buried inside. If δ or ω is too small the random walker may get stuck at the curves and may not be able to cross these singular curves. So a reasonably large number, $0.25 \sim 0.75$, must be chosen as long as the rejection rate is not increased too much.

Another point we want to emphasize is that *the maximality conjecture is destined to be broken.* In order to close an $M-$dimensional volume with concave boundaries we need at least $(M+1)$ cusps. For example, 3 cusps for a two dimensional volume, 4 for three, etc. If there are less than $(M+1)$ cusps then portions of the boundaries must be convex. For example, if we have two cusps for a two dimensional volume then we can make a banana shape at best instead of a concave triangle. For a Lie group the dimension of a representation is unlimited whereas the number of maximal isotropy groups is limited. Thus we have less than the minimal number of cusps and we will see convex boundaries, which means the breaking of the maximality conjecture. That is why we see a convex boundary in Fig. 2.

In conclusion, we have devised a general and robust Monte Carlo algorithm for finding the symmetry breaking directions. The method can be widely used both for the Higgs potential and the Landau potential. Applying it to the Landau theory of the $d-$wave superconductivity, we found that three four-fold symmetries are possible at low temperatures, which agrees with the experiment done on $Tl_2Ba_2CuO_{6+\delta}$ [15].

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FIGURE CAPTIONS

Fig. 1 A random sampling of the orbit space: (θ, ϕ).
Fig. 2 A random sampling of the orbit space: (ϕ, ξ).

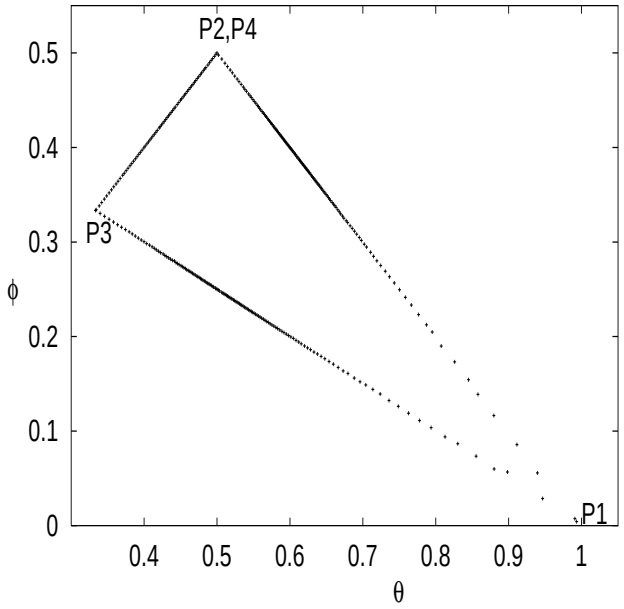

FIG. 1. A random sampling of the orbit space: (θ, ϕ).

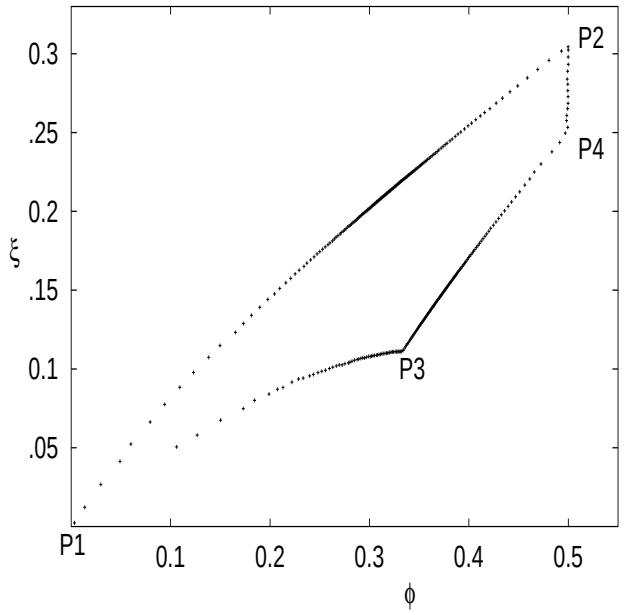

FIG. 2. A random sampling of the orbit space: (ϕ, ξ).